$U(1)$ symmetry breaking in one-dimensional Mott insulator studied by the Density Matrix Renormalization Group method

Isao Maruyama, Tetsuji Koide and Yasuhiro Hatsugai

Department of Applied Physics, University of Tokyo, Hongo Bunkyo-ku, Tokyo 113-8656, Japan

A new type of external fields violating the particle number preservation is studied in one-dimensional strongly correlated systems by the Density Matrix Renormalization Group method. Due to the U(1) symmetry breaking, the ground state has fluctuation of the total particle number, which implies injection of electrons and holes from out of the chain. This charge fluctuation can be relevant even at half-filling because the particle-hole symmetry is preserved with the finite effective field. In addition, we discuss a quantum phase transition obtained by considering the symmetry-breaking fields as a mean field of interchain-hopping.

I. INTRODUCTION

Doped Mott insulators is one of possible candidates of superconductors with electron-electron correlation. At a rational filling, strong electron-electron interaction makes electrons localized in real space. This is the Mott insulator where charge excitations are gapped. Even at this rational filling, the spin degree of freedom survives as a gapless mode where quantum objects as collection of the $S = 1/2$ spins form a singlet ground state.

When mobile carriers are introduced into the Mott insulator, we may expect that the charge gap is destroyed which realizes the superconducting ground state driven by the electron interaction. In the resonating valence bond (RVB) picture proposed by Anderson to describe high-T_c superconducting cuplates[1, 2], doped holes itinerate in a spin-singlet ground state and condense into a superconducting state. If there is no doped hole, i.e., half-filled case, the spin-singlet ground state is expected as a Mott insulator.

Apart from real doping, that is, changing chemical potential, there can be several possibilities for the effective carrier doping. One of a natural possibility can be geometrical frustration in layered organic superconductors, which is approximated by a half-filled Hubbard model with next-nearest-neighbor hopping[3]. Another one is gossamer superconductivity by Laughlin [4]. Even at the half-filed case, finite double occupancy may destroy the Mott insulator at a small on-site Coulomb repulsion and lead the ground state to the gossamer superconducting state[5, 6]. This theory has been also applied to organic superconductors[7]. The gossamer superconducting state is realized not as a ground state of strongly correlated system but a variational function based on a Bardeen Cooper Schrieffer (BCS) superconducting state. However, it can be an exact ground state of the model Hamiltonian [4] which violates the charge conservation as the BCS Hamiltonian. It is thus theoretically interesting to consider $U(1)$ symmetry breaking generically.

Let us recall the BCS Hamiltonian. The BCS Hamiltonian with quadratic terms $\Delta_k c_{k\uparrow}^\dagger c_{-k\downarrow}^\dagger$ has been widely accepted as a theoretical model for superconductors,

where Δ_k is a mean field of pair annihilation amplitude $\langle c_{k\uparrow} c_{-k\downarrow} \rangle$ and $c_{k\sigma}$ are annihilation operators of Fermion. The mean field violates the $U(1)$ gauge symmetry, i.e., the total particle number is not preserved but fluctuating. This charge fluctuation turns out to diverge in the thermodynamic limit[8].

The most simple candidate of $U(1)$ symmetry breaking terms is $\Delta_k c_k^\dagger + h.c.$, which implies injection of electrons and holes from out of the system. The concept of this term is directly connected to local charge fluctuation or doping. Although the previous study is limited to free fermion, such a 1D system defined as $H = \sum_k k c_k^\dagger c_k + \Delta \sum_k (c_k^\dagger + c_k)$ has been studied and was solved with a Jordan-Wigner transformation[9] and with a canonical transformation[10]. To clarify the meaning of Δ, let us describe the procedure of Ref.[9] in detail; this spinless fermion chain can be mapped to semi-infinite XY model with a local magnetic field at the boundary. This local magnetic field in the xy plane turns out to be Δ. In Refs. [9, 10], Δ terms were introduced in different contexts. It is a common concept that the Hamiltonian is an effective one after tracing out of some environment.

There are two motivations of the present work. The first is to clarify the properties of strongly correlated systems with nonuniform charge fluctuation. Especially, a particle-hole symmetric Hubbard model with Δ will make it possible to realize the ground state which is a linear combination of half-filled Mott insulating state with electron-doped and hole-doped states, which evokes the gossamer theory. It is interesting to evaluate fluctuation of total particle number as a direct effect of the $U(1)$ symmetry breaking. The other is to test a mean-field type approach for the interchain hopping of fermion chains. When we consider a decoupling of interchain hopping $t_\perp c_{i\sigma}^\dagger c_{\perp i\sigma}$ into $\Delta_{i\sigma} c_{i\sigma}^\dagger$ with the mean-field type approximation, the effective fields $\Delta_{i\sigma}$ can be identified as $\langle t_\perp c_{i\sigma} \rangle$.[22] In this approach, the Hamiltonian is considered as an effective one obtained after tracing out neighboring chains in the quasi-one-dimensional (quasi-1D) systems.

Since the Hubbard model has Coulomb interaction, we adopt the Density Matrix Renormalized Group (DMRG)

method, which is one of powerful numerical methods for 1D quantum systems[11, 12, 13]. The DMRG method has achieved high precision in various 1D systems while application to two-dimensional lattice is considered to be difficult. As an application to higher dimensions, we note that the DMRG method has already applied to quasi-1D spin systems with interchain couplings as mean fields in the manner of Ref.[14]. This paper may be first attempt to quasi-1D fermionic systems with interchain hopping as mean fields.

The paper is organized as follows. In § II we construct a Hamiltonian with a generalized $U(1)$ breaking term and mention a "bath" site introduced by the canonical transformation[10]. In §III, we describe an application of the DMRG method to the Hamiltonian which does not conserve particle number. In §IV, we demonstrate the mean-field type approach for quasi-1D strongly correlated electron systems. Finally we conclude the results and discuss problems of the mean-field type approach. In Appendix, the note for the canonical transformation is summarized.

II. CORRELATED ELECTRON SYSTEMS WITH $U(1)$ SYMMETRY BREAKING TERM

Let us define a Hamiltonian with the generalized symmetry breaking term term H_Δ

$$H = H_0 + H_\Delta, \tag{1}$$

where H_0 can be one of the Hamiltonians for correlated electrons systems. In this paper we will restrict H_0 to the Hubbard model defined as

$$H_0 = -t \sum_{i=1}^{L-1} \sum_\sigma c_{i+1,\sigma}^\dagger c_{i\sigma} + h.c.$$
$$+U \sum_{i=1}^L \left(n_{i\uparrow} - \frac{1}{2} \right) \left(n_{i\downarrow} - \frac{1}{2} \right) \tag{2}$$

where $c_{i\sigma}$ are fermion operators and L is the system size. The symmetry breaking term H_Δ is defined as

$$H_\Delta = \sum_{i\sigma} \Delta_{i\sigma}^* c_{i\sigma} + \Delta_{i\sigma} c_{i\sigma}^\dagger \tag{3}$$

where $\Delta_{i\sigma}$ are considered as external fields at this stage. This model with nonzero $\Delta_{i\sigma}$ breaks the particle number conservation because H_Δ is not commutable with the total number of particles: $[H_\Delta, N_{tot}] \neq 0$, where $N_{tot} = \sum c_{i\sigma}^\dagger c_{i\sigma}$. This comes from the fact that H_Δ breaks the $U(1)$ symmetry, where the global $U(1)$ rotation defined as $c_{i\sigma} \to e^{i\theta} c_{i\sigma}$.

Generally, external fields break some symmetry as magnetic fields break spin rotational symmetry. In addition to the $U(1)$ symmetry-breaking, H_Δ also breaks the $SU(2)$ spin-rotational symmetry, while the Hubbard model without magnetic field is an $SU(2)$ invariant. The

global $SU(2)$ rotation is defined as $\boldsymbol{c}_i \to U\boldsymbol{c}_i$, where ${}^t\boldsymbol{c}_i = {}^t (c_{i\uparrow}, c_{i\downarrow})$ and $\det U = 1$. The symmetry breaking term transforms under the $SU(2)$ rotation as

$$H_\Delta(\boldsymbol{\Delta}_i) = \sum_i \boldsymbol{c}_i^\dagger \boldsymbol{\Delta}_i + \boldsymbol{\Delta}_i^\dagger \boldsymbol{c}_i$$
$$\to H_\Delta' = H_\Delta(U^\dagger \boldsymbol{\Delta}_i),$$

where ${}^t\boldsymbol{\Delta}_i = {}^t (\Delta_{i\uparrow}, \Delta_{i\downarrow})$. The symmetry is recovered only if $\Delta_{i\sigma} = 0$ for all i, σ.

A. Particle-Hole Symmetry

Let us suppose that H_0 satisfies the particle-hole symmetry, i.e., H_0 is invariant under the usual particle-hole transformation on the tight-binding model: $c_{i\sigma} \to (-1)^i c_{i\sigma}^\dagger$. In other words, H_0 is commute with a anti-unitary operator Θ[15], defined as $\Theta = KU_{ph}$, where K is a complex conjugation and U_{ph} is the unitary operator defined as $U_{ph} = {}_1{}^L \prod_{i\sigma} (c_{i\sigma} + (-1)^i c_{i\sigma}^\dagger)$. It satisfies

$$\Theta^{-1} c_{i\sigma} \Theta = U_{ph}^{-1} c_{i\sigma} U_{ph} = (-1)^i c_i^\dagger,$$

and one can show

$$\Theta^{-1} H_0 \Theta = H_0,$$
$$\Theta^{-1} H_\Delta(\boldsymbol{\Delta}_i) \Theta = H_\Delta \left((-1)^i \boldsymbol{\Delta}_i \right),$$

where t can be complex here and will be fixed $t = 1$ as the unit of energy in numerical calculations. The symmetry-breaking term H_Δ with $\boldsymbol{\Delta}_i = (-1)^i \boldsymbol{\Delta}_i$ is also invariant under the particle-hole transformation. Then, one can construct a Hamiltonian $H = H_0 + H_\Delta$ which preserves the particle-hole symmetry but breaks $U(1)$ and $SU(2)$ symmetries. It is easy to show total number of electrons of this Hamiltonian is half filled when the ground state is unique. The proof is following: because of the particle-hole symmetry $\Theta^{-1} H \Theta = H$, $\Theta^{-1}|gs\rangle$ is also the ground state: $H\Theta^{-1}|gs\rangle = E_{gs}\Theta^{-1}|gs\rangle$. Since the ground state is unique, $|gs\rangle$ is equal to $\Theta^{-1}|gs\rangle$ except for a phase factor. Then one gets

$$\langle gs|N_{tot}|gs\rangle = \langle gs|\Theta^{-1} N_{tot}\Theta|gs\rangle, \tag{4}$$

and N_{tot} satisfies

$$\Theta^{-1} N_{tot} \Theta = 2L - N_{tot}. \tag{5}$$

From eqs.(4) and (5), it is deduced that total number of electrons is half filled, $\langle N_{tot}\rangle = L$. It might be interesting to remind the reader that the half-filled Hamiltonian with the $U(1)$ symmetry breaking term has some analogy to a finite double occupancy in the half-filled case discussed in the gossamer superconducting theory proposed by Laughlin[4].

B. Hidden even-odd Parity conservation

To handle the fermion sign especially by the DMRG which will be discussed in the next section, let us consider a following extension of the Hilbert space by the canonical transformation [10]:

$$c_{i\sigma} \to \tilde{c}_{i\sigma} = (\alpha + \alpha^\dagger)c_{i\sigma},$$

where α is additional annihilation operator of a spinless fermion and satisfies

$$\{\alpha, c_{i\sigma}\} = 0, \quad \{\alpha^\dagger, c_{i\sigma}\} = 0.$$

Canonicality of this transformation can be easily shown as $\{\tilde{c}_{i\sigma}, \tilde{c}_{i'\sigma'}\} = -\{c_{i\sigma}, c_{i'\sigma'}\} = 0$ and $\{\tilde{c}_{i\sigma}, \tilde{c}_{i'\sigma'}^\dagger\} = \{c_{i\sigma}, c_{i'\sigma'}^\dagger\} = \delta_{ii'}\delta_{\sigma\sigma'}$. Moreover, when we denote the fermion operators in H_0 as $H_0(\{c_{i\sigma}\})$, H_0 is invariant under this canonical transformation:

$$H_0 = H_0(\{c_{i\sigma}\}) \to \widetilde{H_0} = H_0(\{\tilde{c}_{i\sigma}\}) = H_0(\{c_{i\sigma}\})$$

because H_0 is made of invariant operators like $\tilde{c}_{i\sigma}^\dagger \tilde{c}_{i'\sigma'} = c_{i\sigma}^\dagger c_{i'\sigma'}$. The term $\widetilde{H_\Delta}$, however, is modified as below,

$$H_\Delta \to \widetilde{H_\Delta} = \sum_{i\sigma} \Delta_{i\sigma}^*(\alpha + \alpha^\dagger)c_{i\sigma} + \Delta_{i\sigma}c_{i\sigma}^\dagger(\alpha + \alpha^\dagger).$$

This formula implies that α site is a "environment bath" site in the spirit of the Dynamical Mean Field Theory(DMFT)[16]. Since single fermion operators in H become bilinear, $\widetilde{H}$ conserves a even-odd parity of the total particle number defined below.

The operator of the total particle number N_{tot} is invariant under the transformation, i.e., $\widetilde{N}_{\text{tot}} = N_{\text{tot}}$. The total Hamiltonian $\widetilde{H}$ does not conserve $\widetilde{N}_{\text{tot}}$ nor the total particle number including alpha $\widetilde{N}_\alpha = \widetilde{N}_{\text{tot}} + \alpha^\dagger\alpha$. That is $[\widetilde{H}, \widetilde{N}_\alpha] \neq 0$. We note that such operators with α as $\widetilde{N}_\alpha$ has no correspondent operator, for example, N_α which was defined before the transformation.

The parity operator of $\widetilde{N}_\alpha$ is defined as

$$\widetilde{P} = e^{i\pi\widetilde{N}_\alpha} = e^{i\pi\alpha^\dagger\alpha} \prod_{i\sigma} e^{i\pi c_{i\sigma}^\dagger c_{i\sigma}}, \quad (6)$$

and satisfies $\widetilde{P}^\dagger\widetilde{P} = 1$ and $\widetilde{P} = \widetilde{P}^\dagger$. One can show the even-odd parity of $\widetilde{N}_\alpha$ is conserved, i.e.,

$$[\widetilde{H}, \widetilde{P}] = 0.$$

Since $\widetilde{P}$ is conserved, one can take simultaneous eigen states of $\widetilde{H}$ and $\widetilde{P}$ as

$$\widetilde{H}|\widetilde{\Psi}(E,p)\rangle = E|\widetilde{\Psi}(E,p)\rangle,$$
$$\widetilde{P}|\widetilde{\Psi}(E,p)\rangle = p|\widetilde{\Psi}(E,p)\rangle,$$

where E is eigen energy and p is ± 1, because $\widetilde{P}^2$ is identity as a operator and $\widetilde{P}$ is unitary. The ground
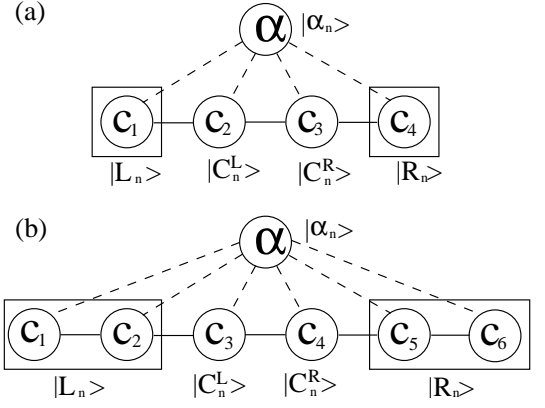

FIG. 1: The system in first iterative procedure for infinite system algorithm of the DMRG with the bath site "α". The system size is enlarged from (a) $L = 4$ to (b) $L = 6$. The α site, left block, center-left site, center-right site and right block are represented by indices $|\alpha_n\rangle, |L_n\rangle, |C_n^L\rangle, |C_n^R\rangle$ and $|R_n\rangle$.

states $|\widetilde{\Psi}(E,p)\rangle$ for $\widetilde{H}$ is doubly degenerated if the ground state $|\Psi(E)\rangle$ for H is unique. As shown in Appendix. A, one can show that expectation value of an arbitrary operator $\mathcal{O}$ can be written as $\langle\Psi(E)|\mathcal{O}|\Psi(E)\rangle = \langle\widetilde{\Psi}(E;+)|\widetilde{\mathcal{O}}|\widetilde{\Psi}(E;+)\rangle = \langle\widetilde{\Psi}(E;-)|\widetilde{\mathcal{O}}|\widetilde{\Psi}(E;-)\rangle$. This means that any expectation value for the system H can be obtained in the system $\widetilde{H}$.

III. METHOD

To study the present 1D strongly correlated system without conservation of the total particle number, the DMRG method is used. As we implied in the previous section, the conservation of even-odd parity of particle number is required to calculate the fermion sign in the DMRG algorithm. In this section we will illustrate detail of the DMRG algorithm and mention the fermion sign. We note that the DMRG method has been applied to the different model which does not conserve total number of particles but conserves it's parity, called the BCS pairing Hamiltonian[17].

First of all, we describe the iterative procedure of the DMRG for the Hamiltonian $\widetilde{H}$ with α site. Figure 1 illustrates systems in first iterative procedure with enlarging the system size from $L = 4$ to $L = 6$. As seen in fig. 1(b), the hopping terms between α site and each sites in $\widetilde{H}_\Delta$ become long range in the successive elongation. Generally speaking, long-range hopping terms such as $c_1^\dagger c_L$ enlarge a numerical error but the numerical error is reduced because the α site is not renormalized in the iterative procedure.

Next, to calculate the fermionic system, one should take care of the fermion sign[12]. When the two local operators $\hat{A}, \hat{B}$ are represented in bases $|A_n\rangle, |B_n\rangle$, one can usually get it's product $\langle A_n B_m|\hat{A}\hat{B}|A_{n'} B_{m'}\rangle =$

$\pm \langle A_n|\hat{A}|A_{n'}\rangle \langle B_m|\hat{B}|B_{m'}\rangle$, where the coefficient $\pm$ is the fermion sign. This formula is valid if the states, $|A_n\rangle$ and $|B_n\rangle$, have a fixed even-odd parity of particle number and operators $\hat{A}, \hat{B}$ conserve the even-odd parity. Otherwise, states or operators are modified. For example such states as $(1+c^{\dagger})|0\rangle$ may change to $(1-c^{\dagger})|0\rangle$ when the states get the fermion sign. This change is hard to followed in the DMRG procedure. This is the reason why conservation of even-odd parity is required by the DMRG.

The canonical transformation makes it possible to calculate the fermion sign because all operators conserve the even-odd parity as shown in eq.(A1) in Appendix. A. Moreover, local bases, $|L_n\rangle$, $|C_n^L\rangle$, $|C_n^R\rangle$, $|R_n\rangle$ and $|\alpha_n\rangle$, have fixed parity as illustrated below.

Then, all local bases in each steps should have fixed even-odd parity of particle number. We explain this with one step of the iterative procedure below.

1. Here we suppose local bases have fixed parity of particle number as in $L = 4$ system.

2. Make the matrix elements of the Hamiltonian $\widetilde{H}$ from local operators represented by local bases, taking care of the fermion sign. The Hamiltonian $\widetilde{H}$ is block diagonalized and has even and odd parity sector.

3. Calculate the ground states $|\widetilde{\Psi}(E_{gs},p)\rangle$ and it's energy E_{gs}, where $p = \pm$ is even-odd parity of particle number.

4. Make the matrix elements of four density matrices $\rho_{L/R,\pm}$;

$$\rho_{L,\pm} = \underset{R,C^R,\alpha}{\mathrm{Tr}}\, \rho_{\pm}, \quad \rho_{R,\pm} = \underset{L,C^L,\alpha}{\mathrm{Tr}}\, \rho_{\pm}, \qquad (7)$$

where $\rho_{\pm} = |\widetilde{\Psi}(E_{gs},\pm)\rangle\langle\widetilde{\Psi}(E_{gs},\pm)|$. One can show that these density matrices are block diagonalized into even and odd parity sector, i.e., $[\rho_{L/R,\pm}, \mathrm{e}^{\imath\pi N_{L/R}}] = 0$, as the Hamiltonian is. We note that if the Hamiltonian conserves particle number, $[H, N_{\mathrm{tot}}] = 0$, the density matrices for the left and right block conserve particle number, $[\rho_{L/R}, N_{L/R}] = 0$.

5. Diagonalize $\rho_{L/R,\pm}$ and select the lowest m eigenvalues and their eigenvectors called renormalized bases, which have fixed parity of particle number because $\rho_{L/R,\pm}$ conserve the parity.

6. Remake matrix elements of all local operators in the renormalized bases. Then, renormalized bases are the next local bases and satisfy the supposition in the step 1.

As described in the procedure, since $\widetilde{H}$ conserves even-odd parity, one can show that each local base in each steps has fixed parity of particle number. That is, one can calculate the fermion sign.

Finally, we note that the number of the states of left and right block is used up to about 60 and the truncation error is less than 10^{-4} in the following results. Since we deal with general $\Delta_{i\sigma}$ which depends on the site, the DMRG method for the random system[18] is employed.

The expectation value is deduced as

$$\langle A \rangle = \frac{1}{2}\sum_{p=\pm}\langle\widetilde{\Psi}(E_{gs},p)|\tilde{A}|\widetilde{\Psi}(E_{gs},p)\rangle, \qquad (8)$$

in order to avoid the numerical error.

IV. RESULTS

In the following, we will show results of a total-charge fluctuation and a particle number in §IV A, which are the direct effect of existence of external fields $\Delta_{i\sigma}$. In §IV B we will show tentative demonstration of the mean-field theory to deal with the interchain hopping.

We note that we restrict the system size L to even to obtain the unique ground state $|\Psi(E)\rangle$ for H. In the DMRG calculation, $\widetilde{H}$ is used and the ground states $|\widetilde{\Psi}(E,p)\rangle$ for $\widetilde{H}$ is doubly degenerated. This degeneracy is artificial due to the canonical transformation.

A. Total-charge fluctuation

When the Hamiltonian H_0 is commutable with $\hat{N}$, the ground state for H_0 has a fixed number of electrons and the total-charge fluctuation, $\Delta N = \sqrt{\langle\hat{N}^2\rangle - \langle\hat{N}\rangle^2}$, is zero when the ground state is unique. On the other hand, since external fields $\Delta_{i\sigma}$ breaks the $U(1)$ symmetry, the total-charge fluctuation becomes finite. The ground state for nonzero $\Delta_{i\sigma}$ becomes a linear combination of electron-doped states and hole-doped states. It implies, even at half-filling, "effective carriers" are introduced by the nonzero $\Delta_{i\sigma}$.

Since large charge gap prefers no fluctuation, when the Coulomb interaction U becomes infinite, doped states are not allowed at half-filling and ΔN becomes zero. In Fig.2, total charge fluctuation ΔN as a function of $1/U$ is plotted as an example of the particle-hole symmetric $\Delta_{i\sigma}$. Infinite U gives no fluctuation $\Delta N = 0$ and finite total-charge fluctuation is proportional to $1/U$. This figure is only for the small system and relatively large $\Delta_{i\sigma}$ but the qualitative character that ΔN is proportional to $1/U$ is general.

It should be noted that maximum of total-charge fluctuation ΔN is order 1 as fig.2 shows $\Delta N \sim \mathcal{O}(1)$ in large $1/U$ region. That is, the present model can not reproduce the BCS ground state with $\Delta N \sim \mathcal{O}(L^{1/2})$. This is important for the charge compressibility defined as $\kappa(\mu) = \frac{\partial n}{\partial \mu} = \frac{1}{L}\frac{\partial\langle N_{\mathrm{tot}}\rangle}{\partial\mu}$. Let us summarize this property for the Mott insulator and the metal: in the Mott insulating state, the charge compressibility diverges at
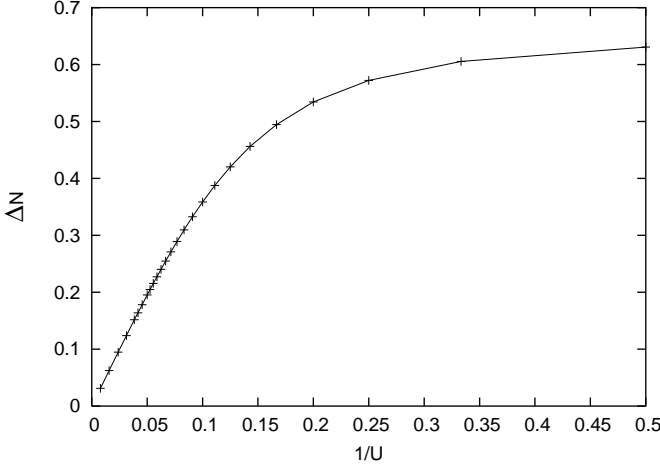
FIG. 2: An example of total charge fluctuation ΔN as a function of $1/U$ for system-size $L = 4$ at half-filling with the Hamiltonian $H = H_0 + H_\Delta$ at $t = 1$ and particle-hole symmetric $\Delta_{n\sigma} = \cos(n\pi/4)$, where $\langle N_{\text{tot}} \rangle = L$ is satisfied numerically. This figure is only for the small system and relatively large $\Delta_{i\sigma}$ but the qualitative character that ΔN is proportional to $1/U$ is general.

$\mu = \pm\Delta_c/2$ and $\kappa(\mu) = 0$ at $-\Delta_c/2 < \mu < \Delta_c/2$, where Δ_c is the charge gap[19]. In the metallic case, the charge compressibility is proportional to the density of states at the Fermi energy. In non-zero $\Delta_{i\sigma}$ case, the charge compressibility at half-filling becomes finite but is expected to become zero at $\mu = 0$ in the limit $L \to \infty$ because the magnitude of ΔN is order $\mathcal{O}(1)$.

B. inter chain hopping as mean fields

In this subsection, let us consider the interchain hopping of 1D Mott insulators. When we take an ansatz of the mean field type, external fields $\Delta_{i\sigma}$ can be determined self-consistently as $-t_\perp c_{i\sigma}^\dagger c_{i_\perp\sigma} \sim c_{i\sigma}^\dagger \Delta_{i\sigma}$. We adopt the self-consistent equation:

$$\Delta_{i\sigma} = -t_\perp \langle c_{i\sigma} \rangle.$$

Although the interchain hopping also gives rise to the effect of the band structure and the dimensionality, the effect of the band structure is not taken into account in this approach. The meaning of $t_\perp$ in the self-consistent equation is the strength of charge fluctuation in the perpendicular direction with the general band structure.

In the DMRG method we used the transformed Hamiltonian, $\tilde{H}$, and the transformed self-consistent equation as $\Delta_{i\sigma} = -t_\perp \langle (\alpha + \alpha^\dagger) c_{i\sigma} \rangle$. We note that $\Delta_{i\sigma}$ is limited to real number for simplicity. In Fig.3 some result of converged $\Delta_{i\sigma}$ after the self-consistent loop for $L = 20$ are plotted. $\Delta_{i\sigma}$ converged smaller value as U increased, which implies a quantum phase transition from nonzero $\Delta_{i\sigma}$ to zero $\Delta_{i\sigma}$.
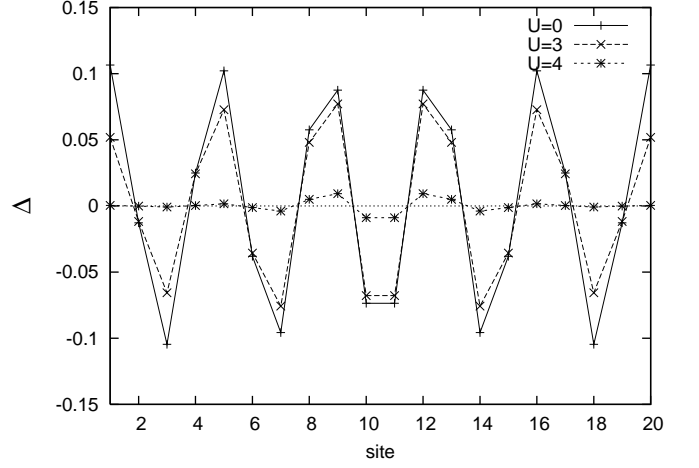

FIG. 3: Converged $\Delta_{i\sigma} = \Delta_i$ as a real function of site i with varying $U = 0, 3, 4$. The system size is $L = 20$.
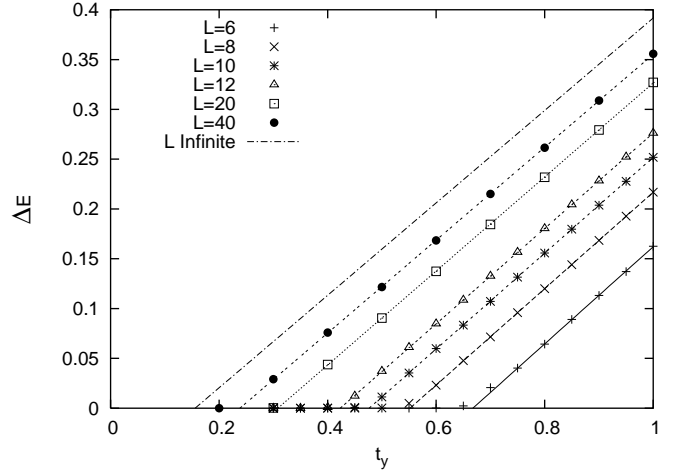

FIG. 4: Stabilization energy $\Delta E = E(0) - E(\Delta_{i\sigma})$ as a function of $t_\perp$ with converged $\Delta_{i\sigma}$ for $U/t = 2$. Points are obtained by the DMRG and lines are fitted with a linear function.

To clarify the transition, one can define the stabilization energy $\Delta E = E(0) - E(\Delta_{i\sigma})$, which means the energy gain due to charge fluctuation in the perpendicular direction, where $E(\Delta_{i\sigma})$ is the ground state energy with converged $\Delta_{i\sigma}$. There are two simple limits: infinite U limit and small $t_\perp$ limit. In both case $\Delta_{i\sigma}$ converged to about zero and the 1D Mott insulator is realized. In Fig.4 the stabilization energy is plotted as a function of $t_\perp$. Increasing $t_\perp$ means that length between chains is changing more closely, which corresponds to applying pressure. In small $t_\perp$ region, ΔE becomes zero, which is identified as the 1D Mott insulator phase. Actually, converged $\Delta_{i\sigma}$ and ΔN are zero there. There is a transition from the 1D Mott insulator phase to the symmetry breaking phase as $t_\perp$ increase. Extrapolated points in Fig.4 show that the transition point $t_\perp^c/t$ is about 0.16 for $U/t = 2$. Since the

charge gap of Mott chain of $U/t = 2$ is $\Delta_c = 0.17$[19], the naive criterion $t_\perp^c \sim \Delta_c$[20] is reasonable in this analysis.

V. CONCLUSION

In conclusion, we have studied the symmetry breaking of $U(1)$ charge and $SU(2)$ spin due to external fields $\Delta_{i\sigma}$, which lead to nonzero total-charge fluctuation ΔN. Finite ΔN means the coherent ground state is a linear combination of electron-doped states and hole doped states. We have applied the DMRG method to the particle-hole symmetric Hubbard chain with $\Delta_{i\sigma}$ and have actually demonstrated that the total-charge fluctuation ΔN at zero-temperature is linear with respect to $1/U$ even at half-filled case $\langle N_{\text{tot}} \rangle = L$.

Considering $\Delta_{i\sigma}$ as a mean field of interchain-hopping tentatively, we have obtained the quantum phase transition from the 1D Mott insulator to the symmetry breaking phase as $t_\perp$ increases, i.e., pressure increases. The transition point $t_\perp^c$ in Fig.4 is close to the charge gap Δ_c. In the symmetry breaking phase, effectively doped carriers itinerate between chains because of non-zero $\Delta_{i\sigma}$. Since the difference between two phases is whether the interchain hopping becomes relevant or not, one may say this transition deconfinement transition[20]. However, since this approach is limited to small $\Delta_{i\sigma}$, clarification of the symmetry breaking phase is remained as future work. The clarification is interesting work because it is well known that destroying the Mott phase by applying the pressure, i.e., increasing $t_\perp$, is typical for high-T_c cuprates.

As described in §IV, the magnitude of ΔN as a function of the system size is constant while the BCS theory gives $\Delta N \sim \mathcal{O}(L^{1/2})$. This property may be related to the fact that we dropped the anti-commutation relation between $\Delta_{i\sigma}$ and fermion operators in the Hamiltonian. That is, expectation value $\langle c_{i\sigma} \rangle$ was a fermionic operator before taking the average as a mean-field. As pointed out in ref. [21], this fact gives the limitation of this "mean field" approach. We can find the another way to bosonize the mean field and this result will be reported in future work.

As a technical outlook, we have used only the infinite method of the DMRG in the self-consistent calculation. The combination of finite method and self-consistent loop will improve the cost of calculation time, where self-consistent field is calculated at center block in sweep of the finite method. In this method, DMRG is combined with the mean-field theory more closely.

Acknowledgments

APPENDIX A: CANONICAL TRANSFORMATION

To summarize properties of the canonical transformation, we introduce the majorana fermions defined as

$$\begin{aligned} \alpha_+ &= \alpha + \alpha^\dagger \\ \alpha_- &= -\imath(\alpha - \alpha^\dagger), \end{aligned}$$

which are unitary and Hermite and satisfy anti-commutation relations $\{\alpha_+, \alpha_-\} = 0$, $\{\alpha_\pm, c_{i\sigma}\} = 0$. It can be proved that even-parity of $\widetilde{P}$ defined in eq.(6) is anti-commutable with α_-: $\{\widetilde{P}, \alpha_-\} = 0$. In addition, the canonical transformation changes any operator for the system H, denoted by $\mathcal{O}$, into $\widetilde{\mathcal{O}}$ which satisfies

$$[\widetilde{P}, \widetilde{\mathcal{O}}] = [\alpha_-, \widetilde{\mathcal{O}}] = 0, \tag{A1}$$

because $\widetilde{\mathcal{O}}$ consists of $c_{i\sigma}, c_{i\sigma}^\dagger$ and α_+, not of α_- and the operator as a polynomial function of fermion operators does not have terms of odd degree. Finally, since the transformation is canonical and the new vacuum is defined as $c_{i\sigma}|\widetilde{0}\rangle = \alpha|\widetilde{0}\rangle = 0$, it can be shown that

$$\langle 0|\mathcal{O}|0 \rangle = \langle \widetilde{0}|\widetilde{\mathcal{O}}|\widetilde{0} \rangle. \tag{A2}$$

To define the canonical transformation of the states, we define bases explicitly as

$$|I\rangle := |\{n_i\}\rangle = \prod_{i=1}^{2L}(c_i^\dagger)^{n_i}|0\rangle. \tag{A3}$$

After the canonical transformation, the bases are written as

$$|\widetilde{I}\rangle := |\widetilde{\{n_i\}}\rangle = \prod_{i=1}^{2L}(\alpha_+ c_i^\dagger)^{n_i}|\widetilde{0}\rangle. \tag{A4}$$

Since $\alpha_\pm^2 = 1$, the bases has even-parity of $\widetilde{P}$: $\widetilde{P}|\widetilde{I}\rangle = |\widetilde{I}\rangle$, where $\widetilde{P}$ is defined in eq.(6). When we define $|\widetilde{I}; +\rangle = |\widetilde{I}\rangle$ and $|\widetilde{I}; -\rangle = \alpha_-|\widetilde{I}\rangle$, one can easily show that a set of 2×4^L bases $|\widetilde{I}; \pm\rangle$ is the ortho-normalized complete set and the bases satisfy $\widetilde{P}|\widetilde{I}; \pm\rangle = \pm|\widetilde{I}; \pm\rangle$ because of $\{\widetilde{P}, \alpha_-\} = 0$.

With eq.(A1) and $\alpha_-^2 = 1$, one can show $\langle \widetilde{I}; +|\widetilde{\mathcal{O}}|\widetilde{I}'; +\rangle = \langle \widetilde{I}; -|\widetilde{\mathcal{O}}|\widetilde{I}'; -\rangle$. With eq.(A2) one can also show $\langle I|\mathcal{O}|I\rangle = \langle \widetilde{I}; +|\widetilde{\mathcal{O}}|\widetilde{I}'; +\rangle$. Combining them, we summarize

$$\langle I|\mathcal{O}|I' \rangle = \langle \widetilde{I}; +|\widetilde{\mathcal{O}}|\widetilde{I}'; +\rangle = \langle \widetilde{I}; -|\widetilde{\mathcal{O}}|\widetilde{I}'; -\rangle. \tag{A5}$$

This means the block diagonalized operator has the same matrix element for even-odd sectors. Since equation (A5)

is true when $\mathcal{O}$ is the Hamiltonian H, the eigen vectors of H and $\widetilde{H}$ can be the same:

$$|\Psi(E)\rangle = \sum_I C_I(E)|I\rangle \qquad (A6)$$

$$|\widetilde{\Psi}(E,\pm)\rangle = \sum_I C_I(E)|\widetilde{I};\pm\rangle, \qquad (A7)$$

where elements $C_I(E)$ satisfy $\langle I|H|I'\rangle C_{I'}(E) = EC_I(E)$.

We note that degenerated eigen vectors $|\widetilde{\Psi}(E,\pm)\rangle$ satisfy $\langle \widetilde{\Psi}(E,p)|\widetilde{\Psi}(E',p')\rangle = \delta_{EE'}\delta_{pp'}$.

We conclude that the expectation value for any operator $\mathcal{O}$ can be written as

$$\begin{aligned}\langle\Psi(E)|\mathcal{O}|\Psi(E)\rangle &= \langle\widetilde{\Psi}(E;+)|\widetilde{\mathcal{O}}|\widetilde{\Psi}(E;+)\rangle \\ &= \langle\widetilde{\Psi}(E;-)|\widetilde{\mathcal{O}}|\widetilde{\Psi}(E;-)\rangle. \quad (A8)\end{aligned}$$

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[22] The limitation of this approach, for example the replacement of a fermionic operator by c-number, is discussed in §V.